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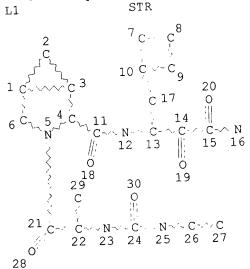
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FILE COVERS 1907 - 15 Sep 2003 VOL 139 ISS 12 FILE LAST UPDATED: 14 Sep 2003 (20030914/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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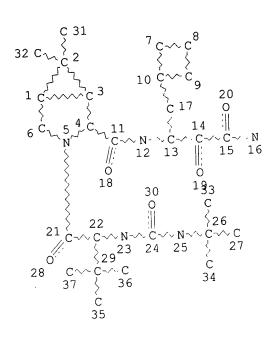
NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

36 SEA FILE=REGISTRY SSS FUL L1 L3

STR L4



NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

13 SEA FILE=REGISTRY SUB=L3 SSS FUL L4 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L5 L6

=> =>

=> d ibib abs hitrn 16 1-2

ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN L6

2003:591204 HCAPLUS ACCESSION NUMBER:

139:149928 DOCUMENT NUMBER:

Preparation of peptides as NS3-serine protease TITLE:

inhibitors of hepatitis C virus

Saksena, Anil K.; Girijavallabhn, Viyyoor M.; Lovey, INVENTOR(S):

Raymond G.; Jao, Edwin; Bennett, Frank; McCormick, Jinping L.; Wang, Haiyan; Pike, Russell E.; Bogen, Stephane L.; Chan, Tin-yau; Liu, Yi-tsung; Zhu, Zhaoning; Njoroge, George F.; Arasappan, Ashok; Parekh, Tejal; Ganguly, Ashit K.; Chen, Kevin X.; Venkatraman, Srikanth; Vaccaro, Henry A.; Pinto, Patrick A.; Santhanam, Bama; Kemp, Scott Jeffrey; Levy, Odile Esther; Lim-Wilby, Marguerita; Tamura, Susan Y.; Wu, Wanli; Hendrata, Siska; Huang, Yuhua;

Wong, Jesse K.; Nair, Latha G. Schering Corporation, USA; Corvas International, Inc. PATENT ASSIGNEE(S):

PCT Int. Appl., 633 pp. SOURCE:

CODEN: PIXXD2

Patent DOCUMENT TYPE:

LANGUAGE:

GΙ

t-Bu

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

											•						
PA	PATENT NO.				KIND DATE				AI	PPLIC	CATIO). I	DATE				
— - WС) 2003 W:	AE, CO, ID,	AG, CR, IL,	AL, CZ, IN,	AM, DE, IS,	AT, DK, JP,	AU, DM, KG,	DZ, KR,	EC, KZ,	EE, LC,	ES, LK,	FI, LR, RO,	GB, LT, RU,	20030 BZ, GD, LU, SC, ZA,	GE, LV, SE,	MA, SG,	MD, SK,
		BY, GH, CH, NL, ML,	KG, GM, CY, PT, MR,	KZ, KE, CZ, SE, NE,	MD, LS, DE, SI,	RU, MW, DK, SK, TD,	TJ, MZ, EE, TR,	SD, ES, BF,	SL, FI, BJ,	SZ, FR, CF,	TZ,	UG, GR, CI,	ZM, HU, CM,	ZW, IE,	AT, IT, GN,	BE, LU, GQ,	BG, MC,
	PRIORITY APPLN. INFO.: OTHER SOURCE(S):					MARPAT 139:149928											

The invention discloses novel peptides I [Y is alkyl, alkylaryl, heteroalkyl, heteroaryl, aryl- or alkylheteroaryl, cycloalkyl, alkyloxy, alkylaryloxy, aryloxy, heteroaryloxy, heterocycloalkyloxy, cycloalkyloxy, alkylamino, arylamino, alkylarylamino, arylamino, heteroarylamino, alkylamino, or heterocycloalkylamino; R1 is acyl; Z is selected from cycloalkylamino, or heterocycloalkylamino; R1 is acyl; Z is selected from O, N, CH or CR; R, R2-R4 are H, alkyl, alkenyl, cycloalkyl, heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate, urea, ketone, aldehyde, cyano, nitro, halo, (cycloalkyl)alkyl, or (heterocycloalkyl)alkyl; W, Q, G, J, L, M independently may be present or absent; W is CO, CS, C(:N-CN), or SO2; Q independently may be present or absent; W is O, CH, alkylidene, NR, S, is CH, N, P, alkylidene, O, NR, S, or SO2; A is O, CH, alkylidene, NR, S,

SO2, or a bond; E is CH, N, alkylidene, or a double bond; G is alkylidene; J is alkylidene, SO2, NH, NR, or O; L is CH, CR, O, S, or NR; M is O, NR, S, SO2, or alkylidene (with provisos)] which have HCV protease inhibitory activity as well as methods for prepg. such compds. In another embodiment, the invention discloses pharmaceutical compns. comprising such compds. as well as methods of using them to treat disorders assocd. With the HCV protease. Thus, peptide $\overline{\text{II}}$ was prepd. and showed $\overline{\text{Ki}}$ = 1-100 nM (category A) in the HCV continuous assay.

394730-60-0P 395647-62-8P 569675-49-6P 569675-86-1P 569676-29-5P 569676-30-8P 569677-40-3P 569677-41-4P 569677-43-6P 569677-66-3P 569677-85-6P 569678-27-9P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BÍOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides as NS3-serine protease inhibitors of hepatitis C virus)

394735-33-2P TΤ

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of peptides as NS3-serine protease inhibitors of hepatitis C virus)

ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN

2002:90062 HCAPLUS ACCESSION NUMBER:

136:167698 DOCUMENT NUMBER:

Preparation of peptides as NS3-serine protease TITLE:

inhibitors of hepatitis C virus

Saksena, Anil K.; Girijavallabhan, Viyyoor Moopil; INVENTOR(S): Lovey, Raymond G.; Jao, Edwin E.; Bennett, Frank;

McCormick, Jinping L.; Wang, Haiyan; Pike, Russell E.; Bogen, Stephane L.; Chan, Tin-Yau; Liu, Yi-Tsung; Zhu,

Zhaoning; Njoroge, F. George; Arasappan, Ashok; Parekh, Tejal N.; Ganguly, Ashit K.; Chen, Kevin X.; Venkatraman, Srikanth; Vaccaro, Henry A.; Pinto, Patrick A.; Santhanam, Bama; Wu, Wanli; Hendrata, Siska; Huang, Yuhua; Kemp, Scott Jeffrey; Levy, Odile

Esther; Lim-Wilby, Marguerita; Tamura, Susan Y.

Schering Corporation, USA; Corvas International, Inc.

PATENT ASSIGNEE(S): PCT Int. Appl., 536 pp.

SOURCE: CODEN: PIXXD2

Patent DOCUMENT TYPE: English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	rent 1	KIND DA		DATE	DATE			APPLICATION NO.					DATE				
	2002008244 W: AE, AG,		AS AL,	AM,		0619 AU,	117	BA,	BB,	F1.77	BR, FI,	BY,	UD,	CA, GE,	- ,		
		ID, MG, TJ,	IL, MK, TM,	IN, MN, TR,	IS,	JP, MZ, TZ,	KG,	KK,	KZ,	ъс, PT.	RO.	RU.	SE,	SG,	SI,	SK,	SL,
	R₩:	GH,	T) TZ	KE,	UΤ	MW, FR, CM,	GB, GA,	GR, GN,	GQ,	11,	ML,	MR,	NE,	/	TD,	TG	CY, BF,
RR	2001 2001 2003 Y APF	0769 0125 0002	88 40 72	A A A	5	2002	0205 0624		A E N	R 20 IO 20 !000-	01-7 01-1 03-2	0900 2540 72		2001 2001 2003 2000	0719 0120		

20010719 WO 2001-US22678 W

OTHER SOURCE(S): GI

MARPAT 136:167698

Peptides I were prepd. wherein Y is alkyl, alkyl-aryl, heteroaryl, heteroalkyl, heteroaryl, aryl-heteroaryl, alkylheteroaryl, cycloalkyl, AΒ alkyloxy, alkylaryloxy, aryloxy, heteroaryloxy, heterocycloalkyloxy, cycloalkyloxy,, alkylamino, arylamino, alkylarylamino, arylamino, heteroarylamino, cycloalkylamino and heterocycloalkylamino; R1 is acyl, borate; Z is selected from O, N, CH or CR; W, Q, G, J, L, M independently maybe present or absent; W is C=O, C=S, C(=N-CN), or SO; Q is CH, N, P, alkylidene, O, amine, S, or SO; A is O, CH, alkylidene, amine, S, SO or bond; E is CH, N, alkylidene, or double bond; G is alkylidene; J is alkylidene, SO, NH, NR, O; L is CH, alkylidene, O, S or NR; M is O, NR, S, SO, alkylidene; p is 0 to 6; and R-R4 are independently selected from the group consisting of H; alkyl; alkenyl; cycloalkyl; heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate, urea, ketone, aldehyde, cyano, nitro, halogen; (cycloalkyl)alkyl and (heterocycloalkyl)alkyl, which have HCV protease inhibitory activity as well as methods for prepg. such compds. In another embodiment, the invention discloses pharmaceutical compns. comprising such compds. as well as methods of using them to treat disorders assocd. With the HCV protease. Thus peptide II was prepd. and tested as antiviral agent and NS3-serine protease inhibitors of hepatitis C virus with Ki ranges in category A = 1-100 nM; category B = 101-1,000 nM; category C > 1000 nM. Also disclosed is the use of I for the manuf. of a medicament for treating HCV, AIDS, and related disorders.

394730-60-0P 395647-62-8P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides as NS3-serine protease inhibitors of hepatitis C virus)

IT

ΙT

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of peptides as NS3-serine protease inhibitors of hepatitis C virus)

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> =>

=> s 15 L7 0 L5

=> =>

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 SEP 2003 HIGHEST RN 585509-69-9 DICTIONARY FILE UPDATES: 14 SEP 2003 HIGHEST RN 585509-69-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L5 ANSWER 1 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN

Page 6 '

569678-27-9 REGISTRY

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-[(1-RNfluorocyclobutyl)methyl]-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-CN dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-(1R, 2S, 5S) - (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C27 H44 F N5 O5 MF

CA SR

CA, CAPLUS STN Files: LC

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1937 TO DATE)

1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 2 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569677-85-6 REGISTRY RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-3,3-dimethyl-1-oxo-2-[[[(2,2,2-trifluoro-1,1-CN dimethylethyl)amino]carbonyl]amino]butyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C27 H42 F3 N5 O5 MF

CA SR

CA, CAPLUS STN Files: LC

1 REFERENCES IN FILE CA (1937 TO DATE) 1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 3 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569677-66-3 REGISTRY

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(2-fluoro-1,1-dimethylethyl)amino]carbonyl]a RN CN mino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C27 H44 F N5 O5 MF

SR CA

CA, CAPLUS STN Files: LC

1 REFERENCES IN FILE CA (1937 TO DATE)

1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 4 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569677-43-6 REGISTRY

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[1-(cyclobutylmethyl)-3-[[[(4-RN methylphenyl)sulfonyl]methyl]amino]-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-CN , (1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C35 H53 N5 O7 S MF

CA SR

CA, CAPLUS LC STN Files:

1 REFERENCES IN FILE CA (1937 TO DATE)

1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 5 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569677-41-4 REGISTRY RN

CN dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C27 H45 N5 O5 MF

SR

CA, CAPLUS STN Files: LC

1 REFERENCES IN FILE CA (1937 TO DATE)

1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 6 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569677-40-3 REGISTRY RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[(1S)-3-amino-1-CN (cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-(1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C27 H45 N5 O5 MF

SR CA

CA, CAPLUS STN Files: LC

1 REFERENCES IN FILE CA (1937 TO DATE) 1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 7 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569676-30-8 REGISTRY RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[1-(cyclobutylmethyl)-3-[[2-[[(1,1-dimethylethyl)methylamino]sulfonyl]ethyl]amino]-2,3-dioxopropyl]-3-CN [(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C34 H60 N6 O7 S MF

SR CA

CA, CAPLUS STN Files: LC

1 REFERENCES IN FILE CA (1937 TO DATE) 1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 8 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569676-29-5 REGISTRY RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[1-(cyclobutylmethyl)-3-[[2-[[(cyclopropylmethyl)amino]sulfonyl]ethyl]amino]-2,3-dioxopropyl]-3-[(2S)-CN 2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C33 H56 N6 O7 S MF

CA SR

STN Files: CA, CAPLUS LC

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1937 TO DATE)

1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 9 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569675-86-1 REGISTRY RN

Glycinamide, N-[[(1,1-dimethylethyl)amino]carbonyl]-3-methyl-L-valyl-(1R, 2S, 5S)-6, 6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carbonyl-.beta.-amino-CN .alpha.-oxocyclobutanebutanoylglycyl-N, N-dimethyl-2-phenyl-, (2S)- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH FS

C39 H59 N7 O7 MF

CA SR

STN Files: CA, CAPLUS LC

. **RELATED SEQUENCES AVAILABLE WITH SEQLINK**

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1937 TO DATE)

1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

ANSWER 10 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

569675-49-6 REGISTRY RN

Glycinamide, N-[[(1,1-dimethylethyl)amino]carbonyl]-3-methyl-L-valyl-(1R, 2S, 5S)-6, 6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carbonyl-.beta.-amino-CN .alpha.-oxocyclobutanebutanoyl-N-(1-methyl-1-phenylethyl)- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH FS

C38 H58 N6 O6 MF

SR CA

CA, CAPLUS STN Files: LC

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1937 TO DATE) 1 REFERENCES IN FILE CAPLUS (1937 TO DATE)

REFERENCE 1: 139:149928

L5 ANSWER 11 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN

RN 395647-62-8 REGISTRY
CN 3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H45 N5 O5

SR CA

LC STN Files: CA, CAPLUS

2 REFERENCES IN FILE CA (1937 TO DATE) 2 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

136:167698 2: REFERENCE

ANSWER 12 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

394735-33-2 REGISTRY

Glycine, N-[[(1,1-dimethylethyl)amino]carbonyl]-3-methyl-L-valyl-RN (1R, 2S, 5S)-6, 6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carbonyl-.beta.-amino-CN .alpha.-oxocyclobutanebutanoyl-, 1-methyl-1-phenylethyl ester (9CI) (CA INDEX NAME)

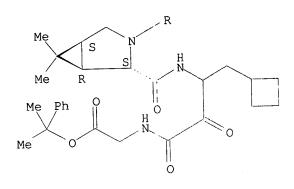
PROTEIN SEQUENCE; STEREOSEARCH FS

C38 H57 N5 O7 MF

SR CA

CA, CAPLUS STN Files: LC

RELATED SEQUENCES AVAILABLE WITH SEQLINK



· 2 REFERENCES IN FILE CA (1937 TO DATE) 2 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

2: 136:167698 REFERENCE

ANSWER 13 OF 13 REGISTRY COPYRIGHT 2003 ACS on STN L5

394730-60-0 REGISTRY RN

3-Azabicyclo[3.1.0]hexane-2-carboxamide, N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-CN dimethyl-1-oxobutyl]-6,6-dimethyl-, (1R,2S,5S)- (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C27 H45 N5 O5 MF

SR CA

CA, CAPLUS LC STN Files:

2 REFERENCES IN FILE CA (1937 TO DATE) 2 REFERENCES IN FILE CAPLUS (1937 TO DATE)

1: 139:149928 REFERENCE

2: 136:167698 REFERENCE